

Computer Physics Communications (2002)

Simple Dynamics for Broad Histogram Method

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Abstract

The purpose of this text is: 1) to clarify the foundations of the broad histogram method, stressing the conceptual differences between it and reweighting procedures in general; 2) to propose a very simple microcanonical dynamic rule, yet to be tested by theoretical grounds, which could provide a good improvement to numerical simulations.

PACS: 75.40.Mg Numerical simulation studies

The broad histogram method (BHM) [1] is based on the exact [2] equation

$$g(E) \langle N_{\text{up}}(E) \rangle = g(E + \Delta E) \langle N_{\text{dn}}(E + \Delta E) \rangle , \quad (1)$$

valid for any system, which is completely general. $g(E)$ counts the number of states sharing the same energy E , and ΔE is a fixed, arbitrary energy jump. Notation $\langle Q(E) \rangle$ stands for the microcanonical average of some quantity Q , i.e. its average over all the above-quoted $g(E)$ states, and only these, uniformly weighted, i.e.

$$\langle Q(E) \rangle = \frac{1}{g(E)} \sum_{i=1}^{g(E)} Q(S_i) . \quad (2)$$

The BHM quantities N_{up} and N_{dn} are computed as follows.

First, one needs to define a protocol of allowed movements, i.e. an agreement concerning the changes to be performed on each state S would be considered, transforming it into

another state S' . Just to fix ideas, think about a system of Ising spins, for which one can agree to perform only single-spin flips, for instance. The only constraint concerning this protocol is reversibility: if $S \rightarrow S'$ is an allowed movement, then $S' \rightarrow S$ is also allowed. For a given state S , $N_{\text{up}}(S)$ simply counts the number of such allowed movements increasing its energy by ΔE , the previously defined fixed jump. Analogously, $N_{\text{dn}}(S)$ counts the number of movements decreasing the energy by the same amount ΔE .

Is the BHM equation really exact and general for any system?

This is a very simple matter: the left-hand side of equation (1) counts the total number of allowed movements from energy level E to energy level $E + \Delta E$; analogously, the right-hand side counts the total number of reverse movements. Reversibility of the protocol gives a positive, definitive answer to the above question.

What has the BHM equation to do with thermodynamics?

Nothing! It concerns only the energy spectrum of the system under study, determined exclusively by its Hamiltonian. No hypothesis was made concerning the particular way the system exchanges energy with the current environment. Nothing to do with ensembles, equilibrium conditions, probabilities, transition rates, detailed balances, temperatures, etc. Of course, $g(E)$ as well as the microcanonical average $\langle Q(E) \rangle$ of any quantity is also independent of these thermodynamic concepts. Even the quoted protocol of movements may have no relation at all with the real movements which would occur under some particular system-environment condition. Would the system be simulated on computers, for instance, the **real** movements performed according to Monte Carlo tossing may be completely distinct from the **virtual** movements counted by N_{up} and N_{dn} . For instance, one can simulate an Ising system through cluster algorithms [3], considering only single-spin flips in order to compute $N_{\text{up}}(S)$ and $N_{\text{dn}}(S)$ for each visited state S , or vice-versa.

How to implement the method?

Suppose one knows the microcanonical averages $\langle N_{\text{up}}(E) \rangle$ and $\langle N_{\text{dn}}(E) \rangle$, as functions of E . Then, equation (1) is used to determine $g(E)$, which is the final goal. Thus, the only remaining task is to find some way (any way) to determine the E -functions $\langle N_{\text{up}}(E) \rangle$ and $\langle N_{\text{dn}}(E) \rangle$. How to perform this task, of course the most important issue, is another story to be discussed later on. Once equation (1) is exact, the numerical accuracy obtained in $g(E)$ depends exclusively on the corresponding accuracies of the inputs $\langle N_{\text{up}}(E) \rangle$ and $\langle N_{\text{dn}}(E) \rangle$.

Note that, until this point, BHM has nothing to do with computer simulations. Alternative approaches could be adopted in order to obtain the microcanonical averages $\langle N_{\text{up}}(E) \rangle$ and $\langle N_{\text{dn}}(E) \rangle$ required by BHM. However, I will restrict the discussion hereafter to this possibility, i.e. to measure these averages from computer simulations.

Even within this restriction, one has many conceivable dynamic rules to choose.

What are the advantages over reweighting methods?

Reweighting methods extract information from the number $V(E)$ of visits to each energy level, during a previously defined Monte Carlo dynamics obeying some detailed balance rule. Thus, the relative visitation frequency to different levels E and E' is previously known, by construction. One example is the histogram method [4] and its further developments [5]. Another example is the multicanonical method [6], which tunes a uniform visitation to all energies. This corresponds to an acceptance rate from E -states to E' proportional to $g(E)/g(E')$: then, by measuring the acceptance rate actually implemented during the computer run, one gets $g(E)$ (apart from an irrelevant multiplicative factor). Other approaches [7] based on this multicanonical idea are also available. Histogram approaches work similarly, by tuning a fixed-temperature, canonical distribution of visits. The two main advantages of BHM over these methods are as follows.

First, fixed-energy, microcanonical averages do not depend on the relative visitation to different energy levels. Only a uniform probability to hit any of the $g(E)$ states sharing the same energy E is required, no matter what are the visits to other energy levels. Thus, in choosing the particular dynamic rule to be adopted, one is not restricted to obey any detailed balance condition, or other similar complications concerning different energy levels. This freedom could be a big advantage, because more adequate dynamic rules could be adopted for each particular application. The only concern is to get a uniform visitation **inside** each energy level **separately**. Of course, this may not be an easy task, but at least it is better than to be also forced to obey further restrictions.

In particular, any dynamic rule obeying detailed balance conditions between different energy levels, such as histogram or multicanonical recipes, also assures a uniform visitation inside each energy level separately. Thus, any of them could be used within BHM, simply by measuring $\langle N_{\text{up}}(E) \rangle$ and $\langle N_{\text{dn}}(E) \rangle$ during the computer run. At the end, instead of the particular prescription of the original recipe, one can use equation (1) in order to obtain $g(E)$. The results cannot be worse than those obtained by the original method, once no further sources of inaccuracies are introduced.

Second, BHM accuracy is indeed better, when **the same** set of averaging states obtained by multicanonical recipes, for instance, is adopted [8]. The reason for that is simple: within reweighting methods, only the actually tossed movement transforming the current state S into the next one is considered, whereas BHM takes into account **all potential** movements one could conceive, starting from S . Similarly, from each state, the information extracted by BHM resides on the **macroscopic** quantities N_{up} and N_{dn} , whereas reweighting methods simply count one more state, $V(E) \rightarrow V(E) + 1$. Within

BHM, $V(E)$ plays no role: it must only be large enough to provide a good statistics. Moreover, this advantage becomes even larger for larger systems, once N_{up} and N_{dn} scale with the system size, at least.

Concluding this part, one possible way to implement BHM is to adopt, for instance, one of the many available multicanonical dynamics, or any other obeying some detailed balance condition (perhaps, [9] is the best one) in order to measure the BHM quantities $\langle N_{\text{up}}(E) \rangle$ and $\langle N_{\text{dn}}(E) \rangle$. Then, $g(E)$ can be obtained by the exact and general BHM relation (1), with better accuracy than that corresponding to exploring the profile of $V(E)$. Obeying detailed balance, the required uniformity of visits within each energy level is assured. Indeed, this approach was followed in many recently introduced methods [10], all of them based on the BHM quantities $\langle N_{\text{up}}(E) \rangle$ and $\langle N_{\text{dn}}(E) \rangle$. However, this corresponds to an effort larger than one needs, because no detailed balance between different energy levels is required by BHM. Another possibility is to profit from that feature by adopting new dynamic rules which provide a uniform visitation within each energy level separately. In other words, by relaxing all restrictions concerning the relative visitation to different energy levels, more efficient computer simulations could emerge. The corresponding dynamic rules remain to be invented. Hereafter, I will briefly treat such an attempt, still on the way.

How to assure a uniform visitation inside a given energy level?

My approach to this question is very naive. Consider some ergodic protocol of allowed movements (again, nothing to do with the BHM protocol of virtual movements). By tossing random movements within this protocol, one can construct a Markov chain by simply accepting any new tossed state, no rejections, no probabilities. Certainly, there is no bias at all: any state among the whole space of states will be reached according to the same probability. Thus, for other rules, I conclude that any bias comes from rejections one is forced to introduce, otherwise the system would stay forever near the maximum entropy region of the energy spectrum. On the other hand, for BHM implementations, one does not need complete uniformity, only within the particular energy level where averages are measured. My naive idea is to completely avoid rejections **within** the particular energy level E currently subjected to the averaging process, although tolerating some rejections out of it. For that, I decided to try the following simple rule [11]: to accept any tossed movement which keeps the system inside the window $[E - \delta E, E + \delta E]$, where $\pm \delta E$ is the maximum energy jump allowed by the protocol, rejecting it otherwise. Although the system is allowed to visit other energy levels inside this window, averages are taken **only** when the system visits the central, rejection-free level E . In reality, this rule is not new. It was inspired by a very similar older one [12], introduced for Ising models within another

context.

Preliminary tests for this dynamics were successful for the 32×32 square lattice Ising model [11], for which the complete energy spectrum $g(E)$ is exactly known [13]: I found deviations which decay by increasing the number N of averaged states inside each energy level, as $1/\sqrt{N}$, along 6 decades until the maximum $N \approx 10^{10}$ tested. Here, I present further tests for larger $L \times L$ lattices, for which the complete energy spectra are not published in [13], but the average energy as well as the specific heat is known. Their exact values at the Onsager temperature [14] are shown in table I, to be compared with the values obtained by the current approach. These results seem to indicate that the above-defined dynamics could be approved against the test of scalability, i.e. it also works well for larger systems. Note that, even by decreasing N by a factor of 10 for larger lattices, the deviations seem to remain at the same level. Perhaps this feature is due to the macroscopic character of $\langle N_{\text{up}}(E) \rangle$ and $\langle N_{\text{dn}}(E) \rangle$. On the other hand, I am not sure that rejections occurring near the averaging energy level do not introduce any bias. Visits to the central, rejection-free level are fed by movements which start at these neighbouring levels where rejections certainly introduce some biases. Although not averaged, these biases could reflect themselves into the central level. Further tests are necessary, with larger lattices, better statistics and other models. Also, some theoretical work concerning the sampling uniformity within the central level would be welcome.

This dynamic rule also presents other advantages. First, one never compares random numbers with precise probabilities like Boltzmann factors, which is a delicate matter for other dynamics. Here, random numbers are used only in order to toss the next movement to be attempted, for instance the next Ising spin to be flipped or not: the decision to perform it is deterministic. Then, the quality of the random number generator is not crucial. Second, the averaging states are not periodically taken, for instance after each complete lattice sweep, avoiding some extra biases which could be introduced by this periodicity. On the contrary, a new averaging state is taken every time the central level is reached, after some previous random movements. For the square lattice Ising model near the critical region, this event occurs every 40 movements on average, but within large fluctuations. Moreover, this number 40 does not depend on the lattice size, relatively saving computer time for larger lattices.

Concluding this last part, the dynamic rule presented above is a promising candidate to be an unbiased microcanonical simulator. Combined with the broad histogram method, equation (1), it can contribute to improving numerical simulation studies.

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Table

L	32	46	62	90	126
e (BHM)	0.141586	0.143063	0.143937	0.144723	0.145205
exact	0.141585	0.143064	0.143937	0.144718	0.145212
C (BHM)	1.846663	2.028195	2.175960	2.362453	2.528842
exact	1.846768	2.027854	2.176425	2.361582	2.528522

Table I Average energy per site (e) and specific heat (C) for $L \times L$ square lattice Ising model at the Onsager temperature. The number of averaging states per energy level is $N = 10^{10}$ for $L = 32, 46$ and 62 , or $N = 10^9$ for $L = 90$ and 126 .